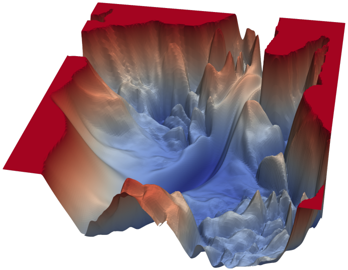
Introduction to Machine Learning

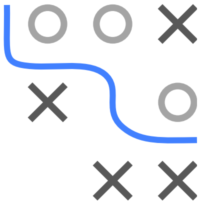
Properties of Loss Functions



Learning goals

- Statistical properties
- Robustness
- Numerical properties
- Some fundamental terminology

THE ROLE OF LOSS FUNCTIONS



Why should we care about the choice of the loss function $L(y, f(\mathbf{x}))$?

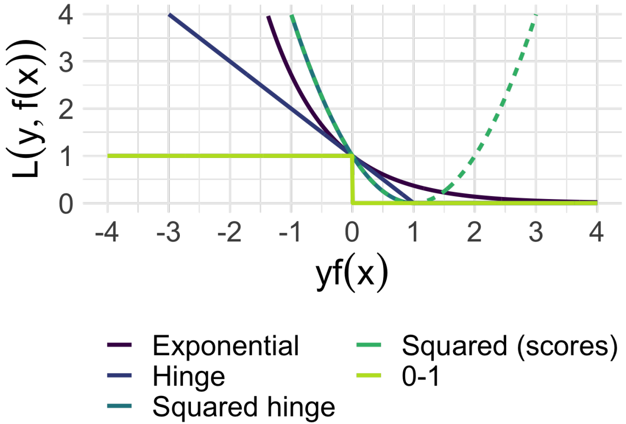
- **Statistical** properties: choice of loss implies statistical assumptions about the distribution of $y \mid \mathbf{x} = \mathbf{x}$ (see *maximum likelihood estimation vs. empirical risk minimization*).
- **Robustness** properties: some loss functions are more robust towards outliers than others.
- **Numerical** properties: the computational complexity of

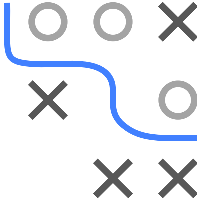
$$\arg\min_{\boldsymbol{\theta} \in \Theta} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$$

is influenced by the choice of the loss function.

SOME BASIC TERMINOLOGY

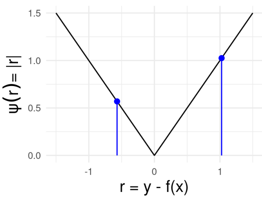
Classification losses are usually expressed in terms of the **margin**:
$\nu := y \cdot f(\mathbf{x})$.



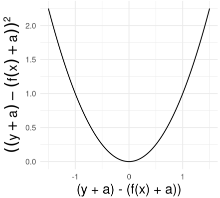


SOME BASIC TERMINOLOGY

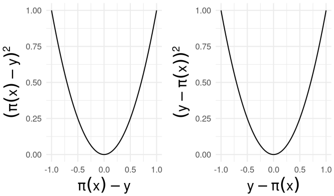
- Regression losses often only depend on the **residuals** $r := y - f(\mathbf{x})$.
- Losses are called **symmetric** if $L\left(y, f(\mathbf{x})\right) = L\left(f(\mathbf{x}), y\right)$.
- A loss is **translation-invariant** if $L(y + a, f(\mathbf{x}) + a) = L\left(y, f(\mathbf{x})\right)$, $a \in \mathbb{R}$.
- A loss is called **distance-based** if
  - it can be written in terms of the residual, i.e., $L\left(y, f(\mathbf{x})\right) = \psi(r)$ for some $\psi : \mathbb{R} \to \mathbb{R}$, and
  - $\psi(r) = 0 \Leftrightarrow r = 0$.



Distance-based: $L1$



Translation-invariant: $L2$



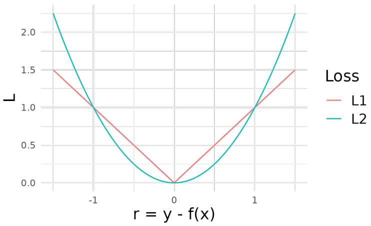
Symmetric: Brier score

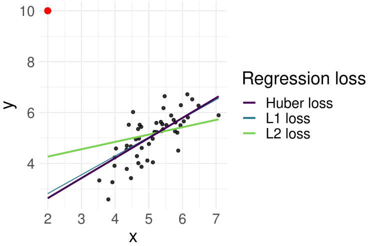
ROBUSTNESS

Outliers (in y) have large residuals $r = y - f(\mathbf{x})$. Some losses are more affected by large residuals than others. If loss goes up superlinearly (e.g. L2) it is not robust, linear (L1) or even sublinear losses are more robust.

$y - \hat{f}(\mathbf{x})$	$L1$	$L2$	Huber ($\epsilon = 5$)
1	1	1	0.5
5	5	25	12.5
10	10	100	37.5
50	50	2500	237.5

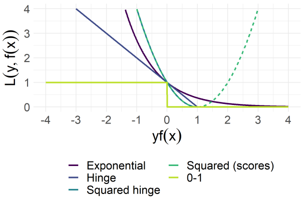
As a consequence, a model is less influenced by outliers than by "in-liers" if the loss is **robust**.
Outliers e.g. strongly influence $L2$.





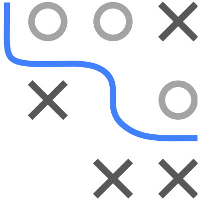
NUMERICAL PROPERTIES: SMOOTHNESS

- **Smoothness** of a function is a property measured by the number of continuous derivatives.
- Derivative-based optimization requires smoothness of the risk $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$
  - If loss is unsmooth, we might have to use derivative-free optimization (or worse, in case of 0-1)
  - Smoothness of $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ not only depends on L, but also requires smoothness of $f(\mathbf{x})$!



Squared loss, exponential loss and squared hinge loss are continuously differentiable. Hinge loss is continuous but not differentiable. 0-1 loss is not even continuous.

NUMERICAL PROPERTIES: CONVEXITY



- A function $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ is convex if

$$\mathcal{R}_{\text{emp}}\left(t \cdot \boldsymbol{\theta} + (1 - t) \cdot \tilde{\boldsymbol{\theta}}\right) \leq t \cdot \mathcal{R}_{\text{emp}}\left(\boldsymbol{\theta}\right) + (1 - t) \cdot \mathcal{R}_{\text{emp}}\left(\tilde{\boldsymbol{\theta}}\right)$$

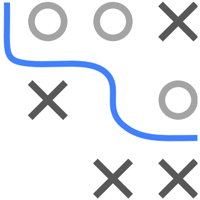
  $\forall\, t \in [0, 1],\ \boldsymbol{\theta}, \tilde{\boldsymbol{\theta}} \in \Theta$
  (strictly convex if the above holds with strict inequality).

- In optimization, convex problems have a number of convenient properties. E.g., all local minima are global.

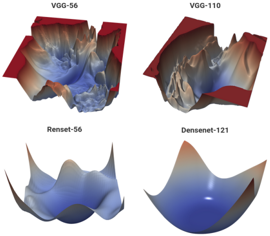
  $\rightarrow$ strictly convex function has at most **one** global min (uniqueness).

- For $\mathcal{R}_{\text{emp}} \in \mathcal{C}^2$, $\mathcal{R}_{\text{emp}}$ is convex iff Hessian $\nabla^2\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ is psd.

NUMERICAL PROPERTIES: CONVEXITY



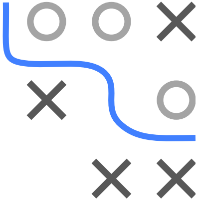
- Convexity of $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ depends both on convexity of $L(\cdot)$ (given in most cases) and $f(\mathbf{x} \mid \boldsymbol{\theta})$ (often problematic).
- If we model our data using an exponential family distribution, we always get convex losses
  - For $f(\mathbf{x} \mid \boldsymbol{\theta})$ linear in $\boldsymbol{\theta}$, linear/logistic/softmax/poisson/... regression are convex problems (all GLMs)!



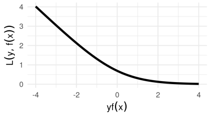
Li et al., 2018: *Visualizing the Loss Landscape of Neural Nets*. The problem on the bottom right is convex, the others are not (note that very high-dimensional surfaces are coerced into 3D here).

NUMERICAL PROPERTIES: CONVERGENCE

In case of **complete separation**, optimization might even fail entirely, e.g.:



- Margin-based loss that is strictly monotonicly decreasing in $y \cdot f$, e.g., **Bernoulli loss**:



$$L\left(y, f(\mathbf{x})\right) = \log\left(1 + \exp\left(-yf(\mathbf{x})\right)\right)$$

- f linear in $\boldsymbol{\theta}$, e.g., **logistic regression** with $f(\mathbf{x} \mid \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \mathbf{x}$
- Data perfectly separable by our learner, so we can find $\boldsymbol{\theta}$:

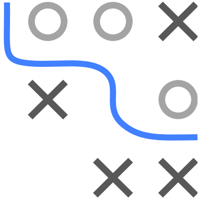
$$y^{(i)} f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right) = y^{(i)} \boldsymbol{\theta}^T \mathbf{x}^{(i)} > 0 \;\; \forall \mathbf{x}^{(i)}$$

- Can now a construct a strictly better $\boldsymbol{\theta}$

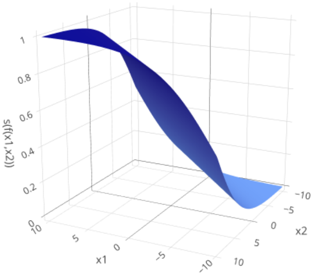
$$\mathcal{R}_{\text{emp}}(2 \cdot \boldsymbol{\theta}) = \sum_{i=1}^{n} L\left(2 y^{(i)} \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right) < \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$$

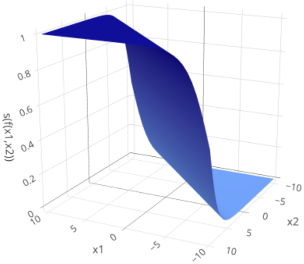
- As $||\boldsymbol{\theta}||$ increases, sum strictly decreases, as argument of L is strictly larger
- We can iterate that, so there is no local (or global) optimum, and no numerical procedure can converge

NUMERICAL PROPERTIES: CONVERGENCE



- Geometrically, this translates to an ever steeper slope of the logistic/softmax function, i.e., increasingly sharp discrimination:





- In practice, data are seldomly linearly separable and misclassified examples act as counterweights to increasing parameter values.
- Besides, we can use **regularization** to encourage convergence to robust solutions.